A second order cartesian scheme for BGK equation

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Abstract. *A simple second order scheme is presented for BGK equation on cartesian grids to simulate rarefied gas flows. An immersed boundary technique is then used since the mesh is body fitted. The asymptotic preserving properties of the BGK equation discretization towards Euler limit are also investigated with emphasis on the boundary conditions as the Knudsen number goes to zero. Reconstruction techniques and levelset functions are used to modify the fluxes at the nearest interface of the body and enforce the boundary conditions at second order. The same method is applied in 1D and 2D cases to demonstrate its accuracy.*

Keywords: BGK model; cartesian meshes; second order.

1 INTRODUCTION

Boltzmann's equation is the main tool for modeling rarefied gas regimes [2]. Different methods exist to solve this equation like Direct Simulation Monte Carlo (DSMC, [1]). It is a statistical method and the results are very noisy. The Lattice Boltzmann method [3] is also used but has issues to simulate flows at high Mach numbers. The BGK model [4] is an other computationally viable approximation of the Boltzmann's equation which provide a simpler expression for the collision term. The BGK equation is the following :

$$\frac{\partial f}{\partial t}(x,\xi,t) + \xi \cdot \bigtriangledown_x f(x,\xi,t) = \frac{1}{\tau}(M_f(x,\xi,t) - f(x,\xi,t)) \tag{1}$$

where f is the density distribution function, x is the space variable, ξ is the velocity variable, τ the relaxation time and M_f the Maxwellian distribution function expressed as:

$$M_f = \frac{\rho}{(2\pi T)^{3/2}} exp(-\frac{|U-\xi|^2}{2T})$$

with ρ the density, U the macroscopic velocity and T the temperature. It corresponds to the density distribution function when the gas is at thermodynamic equilibrium. The source term (or collision term) of the BGK model indicates that the distribution function is relaxed towards the maxwellian. The relaxation time depends on the Knudsen number which is the ratio between the main free path and the characteristic length of the problem. When the Knudsen number goes to zero, the continuum limit is reached and the BGK model tends to the compressible Euler equations. This is a well known property of the model given by the Chapman-Enskog expansion. However, the dependency of the distribution function in space and velocity makes the resolution of the BGK equation computationally intensive compared to the compressible Euler model.

In the proposed presentation we intend to describe a discrete method to take into account wall boundary conditions on a cartesian mesh, i.e., on a grid that is not body fitted. This kind of grid is very suitable for massive parallel computing and does not require a remeshing step for moving geometries. The plan is to recover higher-order accuracy at the border. An additional issue that we consider is the actual boundary condition to be imposed at the solid wall. In order to couple BGK and Euler equations when kinetic and continuum regimes coexist, the numerical method for BGK has to asymptotically preserve the Euler limit at the discrete level when the Knudsen number goes to zero. In particular, when solid walls are present in the flow, the asymptotic preserving properties at the walls are to be ensured. The classic diffusive condition consider the wall at equilibrium with its own temperature, independent of the fluid. It is not asymptotic preserving because of a non-zero energy flux in the limit. Also, naively applying a specular reflection at the boundary requires interpolations of the distribution function and that can create a diffusive layer also when the energy flux has to be zero (as for the impermeability condition). Finer velocity grids or high order interpolations could solve this problem but the computational time dramatically increases.

2 A DISCRETE AP IMPERMEABILITY CONDITION

A new way of applying the impermeability condition for BGK equation at solid boundaries is therefore developed using a fictive state in the solid, as if it was at equilibrium. This fictive state is represented by a maxwellian distribution function defined thanks to macroscopic quantities extrapolated from the fluid (temperature and velocity). The normal component of the velocity used to compute the maxwellian is zero and the density is such that the mass flux through the wall is zero. To do so, one needs the distribution function at the boundary for all microscopic velocities that are going towards the wall. An upwind reconstruction is used to approximate this distribution function. A graphical illustration is shown on Figure 1.

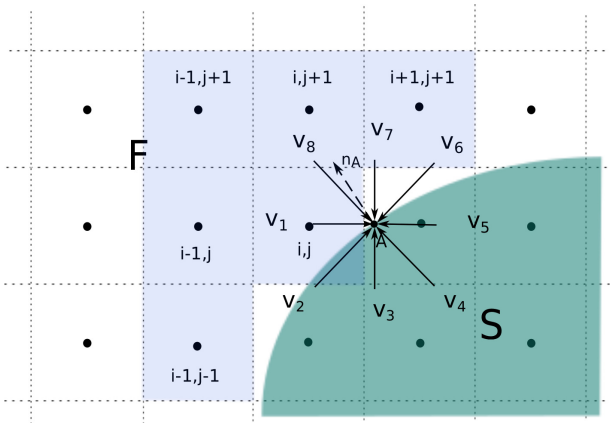

Figure 1: Graphic illustration of the reconstruction

On this example, the distribution function is required for v_1, v_6, v_7, v_8. The values of the reconstructed distribution function $\tilde{f}$ for these four velocities are respectively $f_{i,j}(v_1)$, $f_{i+1,j+1}(v_6)$, $f_{i+1,j+1}(v_7)$, $f_{i,j+1}(v_8)$. The maxwellian M_f is first computed with a density of 1. Imposing a zero mass flux through the boundary gives the real density ρ_w as :

$$\rho_w = \frac{\int_{v.n_A<0} \tilde{f} v.n_A dv}{\int_{v.n_A>0} M_f v.n_A dv} \qquad (2)$$

The maxwellian M_f is then rescaled with this density to get the actual boundary condition used as fictive state.

Once the maxwellian is built at the solid interface, the fluxes in the nearest fluid cell interface to the boundary are modificated to take into account the boundary condition through the fictive state. To improve accuracy, geometrical considerations have to be taken into account like the distance to the body and the outward normal. Such quantities are known through a levelset function that is used to define the body.

When the Knudsen number goes to zero, the relaxation term becomes stiff and treating it explicitly in time requires time steps smaller than the relaxation time (usually the same order of the knudsen number). To avoid stability restriction and keep reasonable time steps, the time discretization is performed by a second order IMEX scheme [5]. It is a Runge-Kutta scheme with different coefficient for each terms. Thus, the stiff part (which is non linear) is treated implicitly while an explicit scheme is used for the convective part which is linear. The non linearity is not an issue because the moments of f and the maxwellian are the same. One can find the macroscopic quantities at the next Runge-Kutta step and build a new maxwellian for the implicit part.
The space discretization is performed using a finite volume method. A MUSCL reconstruction with slope limiters (minmod) is applied to get second order.

3 NUMERICAL RESULTS

In the following preliminary results, errors and convergence rates are investigated with respect to several exact test cases in the continuum regime. Solutions in one and two dimensions are presented.

For a reflection of a 1D rarefaction wave and a 1D shock wave, the L_1, L_2 and L_{inf} errors with respect to the exact solutions are presented for different boundary positions with respect to the grid. The wall is located at x=3 and the grid is moved such that for each grid points x_i, $x_i = x_i + \psi\Delta x$. For $\psi = 0$ and $\psi = 1$ the wall is located on a grid point. In both cases, the error stays close to the optimal error calculated when the boundary is exactly at a grid interface ($\psi = 0.5$). In L_{inf}-norm, oscillations are observed because the maximal error is not always located in the same cell. Also, the error increases as ψ goes to zero due to bigger extrapolation errors.

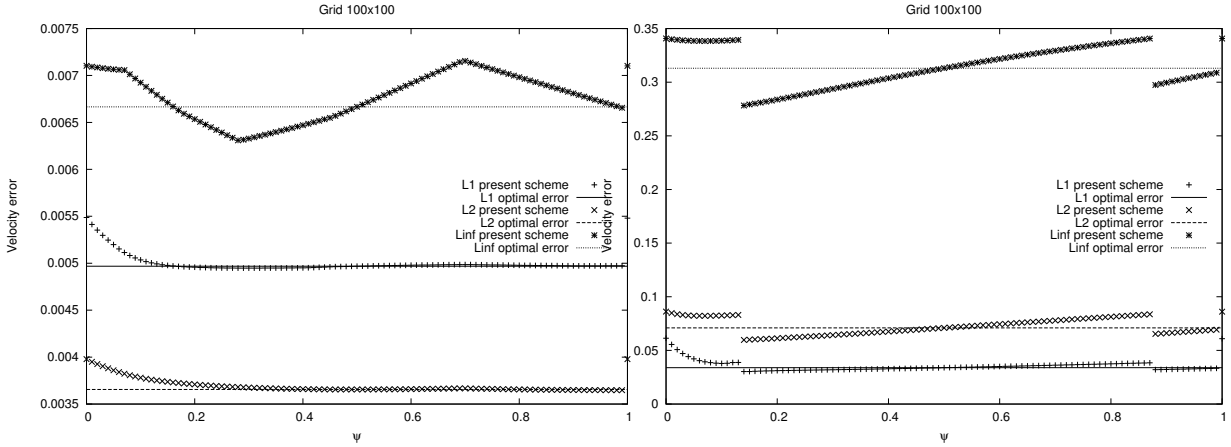

Figure 2: Errors in different norms for the reflection of a rarefaction wave

Figure 3: Errors in different norms for the reflection of a shock wave

The same technique is applied in 2D on the Ringleb flow. This is a potential flow where the analytical solution for Euler equations is known. The solution is calculated between two streamlines considered as walls. Thus, convergence rates with respect to this solution can be computed for the method at a Knudsen number of 10^{-10}. For the velocity along y-axis, the pressure and the speed of sound, convergence order around 2 are obtained (2.06, 1.96, 1.9 respectively).

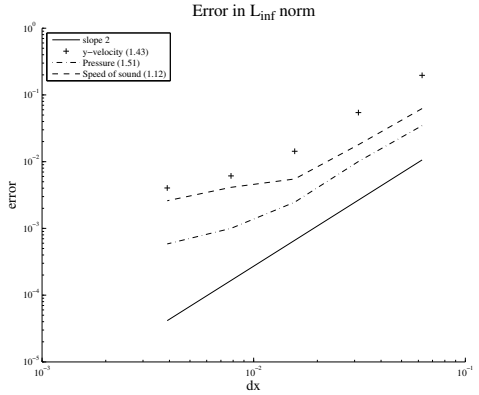

Figure 4: L_{inf} accuracy for the pressure, speed of sound and y-velocity on the Ringleb flow

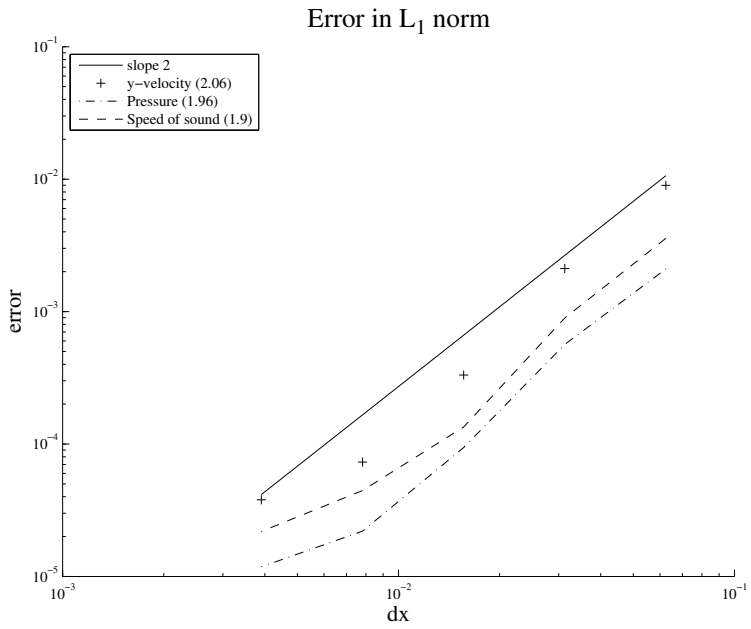

Figure 5: L_1 accuracy for the pressure, speed of sound and y-velocity on the Ringleb flow

4 CONCLUSIONS

A "new" boundary condition has been built satisfying the impermeability condition of Euler equations. The wall is considered at thermodynamic equilibrium and all the macroscopic quantities are extrapolated from the fluid. Only the normal component of the velocity is enforced to be zero. The 1D and 2D cases presented show that the boundary conditions preserve the compressible Euler asymptotic limit, and that they are imposed with a reasonable degree of accuracy on a cartesian mesh.

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